LA-UR-18-22012
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Title: Actinides and Correlated Electron Materials

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Intended for: Laboratory strategy
Report
Web

Issued: 2018-03-12

LOS ALAMOS NATIONAL LABORATORY

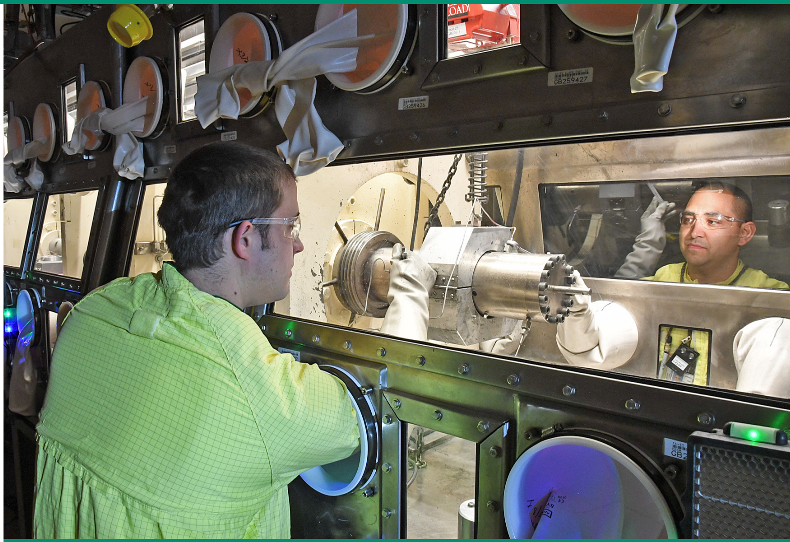
ACTINIDES AND CORRELATED ELECTRON MATERIALS

The Actinides and Correlated Electron Materials area of leadership spans Los Alamos National Laboratory competency in actinide materials research dating to the Manhattan Project as articulated in the *Integrated Plutonium Science and Research Strategy* and competency in strongly correlated electron systems dating back to at least the early 1980s.

This area of leadership focuses on the goals of **discovering, understanding, and controlling emergent electronic states** and **predictive performance of actinide materials**. They are quintessentially linked by the fact that the physics of actinides—and plutonium in particular—are governed by strong electronic correlations. Not only is the electronic structure of actinides dictated by fine details of electron correlations, but chemical bonding and physical structure are as well. Hence, by addressing the first goal of this leadership area we can significantly accelerate progress on the second goal. To understand such matter requires probing the intertwined spin, charge, orbital, and lattice degrees of freedom with greater precision and developing models that accurately predict the consequences of these coupled degrees of freedom, on multiple length and time scales and including acute reactivity and effects of self-irradiation phenomena in these materials.

- **Discover, understand, and control emergent electronic states:** The emphasis here is on tuning the influence of strong correlations, especially in *f*-electron systems, in diverse environments and topologies. Novel functionalities, such as unconventional superconductivity and other quantum states, frequently emerge. The existence of multiple competing or interacting degrees of freedom is common.

- **Predictive performance of actinide materials:** Meeting performance requirements from ambient to extreme conditions with prediction-driven structure-property relationships amidst aging and lifetime issues is a particular challenge with *f*-electron materials. The challenge is two-fold: 1) to forward-predict processing and aging effects on actinide performance that include a quantified uncertainty involving the identification of fundamental control variables (dose, dose rate, temperature); and



An innovative workforce skilled in controlling emergent electronic states and in predicting performance of actinide materials is the foundation of Los Alamos National Laboratory's leadership in actinides and correlated electron materials. Shown are research technicians at work on the 40-mm gun, a key research tool for understanding the dynamic properties of plutonium.

Materials for the Future

The Los Alamos National Laboratory Materials for the Future strategy derives from our vision to support the Laboratory's national security mission drivers.

We pursue the discovery science and engineering for advanced and new materials to intentionally control functionality and predict performance relevant to ensuring the success of the Lab's missions.

To deliver on our missions, our materials strategy builds on materials science and engineering, enabling the necessary Laboratory leadership in seven key areas:

- Complex Functional Materials
- Material Resilience in Harsh Service Conditions
- Manufacturing Science
- Actinides and Correlated Electron Materials
- Integrated Nanomaterials
- Energetic Materials
- Materials Dynamics

2) to develop a science-based framework for quantifying margins and uncertainties actinide materials impact on performance to gauge what we do and do not know (and how well). Understanding plutonium's 5*f* electrons plays a central role in meeting this challenge.

Cross-cutting requirements for both goals include a robust modeling and computational capability spanning multiple length and time scales to allow materials design for functionality and coupling this capability with experiments that probe and map matter across relevant length and time scales to validate predictive models and to provide new understanding.

Los Alamos Leadership in Actinides and Correlated Electron Materials

Los Alamos National Laboratory's leadership in actinides and correlated electron materials is well recognized worldwide. This recognition has grown over the decades from an institutional perspective that its workforce should be of the highest caliber, pursuing cutting-edge research and simultaneously responding to the defense and energy needs of the country. The predictive performance of actinide materials goal is quintessential to the Laboratory's nuclear deterrence mission to ensure predictable performance of the nuclear stockpile in the absence of underground nuclear testing. This goal, however, cannot be realized without the fundamental science underpinning the goal of understanding and controlling emergent electronic states.

Key Science Questions

- How do we understand—and eventually control—the emergent properties of quantum matter, which arise from complex correlations of the atomic or electronic constituents?
- What are the relevant length and time scales for controlling functionality in correlated electron materials in general, and plutonium in specific?
- What is the relevant interplay among structure, topology, correlations, pressure, temperature, magnetic field, strain rate, defects, and interfaces (including surfaces) that gives a specific response, and what is the specific role of the 5*f* electrons?
- What is beyond Fermi liquid theory as a framework for describing interacting electrons?
- Can we predict and control the time-dependent interactions of *f*-electron materials with the environment (e.g., radiation damage [including self irradiation and external sources], interfacial chemistry, and their coupling)?

10-year End State

The ultimate goal of this area of leadership is to discover and control emergent properties for enhanced functionality at the atomic scale, mesoscale, and macroscale; and connect predictive theory to process-, age- and correlation-aware performance for science-based product certification. This includes the ability to predict the aging behavior of plutonium.

To achieve these goals, we envision the establishment of an integrated science capability through collocation, instrumentation development, and strategic partnerships. This integrated capability will have facilities that leverage existing investments—for example, integrating fundamental research activities into the Radiological Laboratory/Utility/Office Building; extending sample environment capabilities at existing facilities; extending synthesis capabilities to plutonium-242, single crystals, and thin films; and developing the highest caliber scientists who understand the problems in both correlated electrons and the predictive performance of plutonium. Growth, characterization, and computational capabilities need to be modernized, and electronic structure models must be improved for validation of experimental results.

To ensure success, strategic partnerships with Lawrence Livermore National Laboratory, Idaho National Laboratory, and the international community will be leveraged through coordination by the Laboratory's G.T. Seaborg Institute for Transactinium Science. Proactive outreach to the user communities of existing programs (Center for Integrated Nanotechnologies, National High Magnetic Field Laboratory, Los Alamos Neutron Science Center) and other national user facilities will provide access to a stream of innovative ideas and position Los Alamos to be the partner of choice for the leading actinide and correlated electron materials community.

For more information, please see materials.lanl.gov or send email to materials@lanl.gov.

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